09/683912

## **WEST Search History**

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DATE: Wednesday, February 11, 2004

Hide?	Set Name	Query	Hit Count	
	DB=PGPB, $USPT$ , $EPAB$ , $JPAB$ , $DWPI$ , $TDBD$ ; $PLUR=YES$ ; $OP=OR$			
	L1	probe adj array	3881	
	L2	interface	809816	
	L3	11 and 12	1119	
	L4	(probe adj array) same interface	109	
	DB=PGPB,	· PLUR=YES; OP=OR		•
	L5	14	(49')	
	DB = USPT;	PLUR=YES; OP=OR		
	L6	L4	50 /	
	DB=EPAB;	PLUR=YES; OP=OR		
	L7	L4	2	
	DB=JPAB;	PLUR=YES; OP=OR	Displaye  W/o P2.	J AB
	L8	L4	0 14 32	
	DB=DWPI	PLUR=YES; OP=OR	,   W/8 /	
	L9	L4	7 7	
	DB = TDBD	; PLUR=YES; OP=OR		
	L10	L4	\ 1 \land \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	

**END OF SEARCH HISTORY** 

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s ((probe (w) array#) 10a (program? (w) interface#))/bi,ab MISSING OPERATOR ARRAY#) 10A The search profile that was entered contains terms or

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s (probe(w)array#0(10a)(program?(w)interfac?)/bi,ab UNMATCHED LEFT PARENTHESIS '(PROBE' The number of right parentheses in a query must be equal to the number of left parentheses.

=> s ((probe(w)array#)(10a)(program?(w)interfac?))/bi,ab 189533 PROBE/BI 163334 PROBE/AB 106261 ARRAY#/BI 99649 ARRAY#/AB 260336 PROGRAM?/BI 213963 PROGRAM?/AB 341069 INTERFAC?/BI 298671 INTERFAC?/AB L1 0 ((PROBE(W)ARRAY#)(10A)(PROGRAM?(W)INTERFAC?))/BI,AB

=> s ((array#)(10a)(program?(w)interfac?))/bi,ab 106261 ARRAY#/BI 99649 ARRAY#/AB 260336 PROGRAM?/BI 213963 PROGRAM?/AB 341069 INTERFAC?/BI 298671 INTERFAC?/AB

L2 1 ((ARRAY#)(10A)(PROGRAM?(W)INTERFAC?))/BI,AB

=> d 2 1 bib ab 1 ANSWERS ARE AVAILABLE. SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE The answer numbers requested are not in the answer set. ENTER ANSWER NUMBER OR RANGE (1):1

L2 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN AN 2003:181689 CAPLUS

TI Using the common component architecture in chemistry AU Windus, Theresa L.; Jurrus, Elizabeth R.; Krishnan, Manojkumar; Nieplocha, Jaroslaw; Janssen, Curtis L.; Bernholdt, David E.; Curfman McInnes, Lois; Sarich, Jason; Benson, Steve CS Molecular Science Software Group, Pacific Northwest National Laboratory, Richland, WA, 99352, USA

SO Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, United States, March 23-27, 2003 (2003), COMP-002 Publisher: American Chemical Society, Washington, D. C. CODEN: 69DSA4

DT Conference; Meeting Abstract LA English

AB Today's computational chem. codes are very complex and can be difficult to interface with other software and libraries. Language interoperability and differences in parallel/programming paradigms are just two examples of some of the problems that are faced. This talk will describe the use of the Common Component Architecture in massively parallel computational chem. In particular, this talk will describe recent

computational chem. In particular, this talk will describe recent work using NWChem interfacing with other software components such as MPQC, TAO, and Global Arrays. NWChem and MPQC are computational chem. software packages, TAO is an optimization package, and Global \*\*\*Arrays\*\*\* is an an efficient and portable

"shared-memory" \*\*\*programming\*\*\* \*\*\*interface\*\*\* for distributed-memory computers.

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